Excitation of heavy hydrogenlike ions in relativistic collisions

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We study the excitation of heavy hydrogenlike ions occurring in high-energy collisions with many-electron atoms by considering three theoretical approaches. In all of them the initial and final undistorted states of the electron in the ion are described by relativistic Coulomb-Dirac wave functions. In two of these approaches the interaction between the electron of the ion and the atom is described within the first order perturbation theory. In the first approach the presence of the atomic electrons is neglected whereas the second approach takes them into account. The comparison of results of these two approaches allows one to establish the range of collision energies where the effect of the electrons of the atom on the excitation process is weak and can be neglected. At these energies, however, the interaction between the electron of the ion and the nucleus of the atom may become too strong for the first order theory to be a good approximation. In order to deal with this point we present the third approach which is based on the symmetric eikonal approximation. Theoretical results are compared with available experimental data.

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I. INTRODUCTION

In ion-atom collisions, where the collision velocity v approaches the speed of light c ($c \approx 137$ a.u.), the colliding particles are exposed to electromagnetic fields which in general substantially differ from fields produced in nonrelativistic collisions. Besides, the internal motion of electrons in very heavy ions is also noticeably influenced by the relativistic effects. All this considerably alters the dynamics of ion-atom collisions which involve heavy ions moving at high velocities compared to results suggested by calculations performed under the assumption that the speed of light is infinite.

During the last two decades there has been accumulated the considerable amount of experimental and theoretical results for the ionization of K shells of heavy atoms in relativistic collisions with pointlike charges (see for a review [1–6] where also a wealth of references to original papers can be found). Besides, more recently there have been substantial efforts devoted to the exploration of the electron loss from heavy ions colliding with atoms at relativistic impact energies (for a review see [7]). The process of the excitation of such ions, however, has been much less studied and both experimental and theoretical results for this process are scarce [6,8,9].

In the present paper we consider the excitation of heavy hydrogenlike ions colliding with neutral many-electron atoms. The paper is organized as follows. The next section (Sec. II) contains the general description of the theoretical approaches which we use to treat the excitation process. In Sec. III these approaches are employed to calculate excitation cross sections. Atomic units are used throughout except where otherwise stated.

II. GENERAL

The collision between an ion carrying an electron and an atom involves at least four particles. A rigorous and comprehensive treatment of such a collision in the domain of relativistic impact energies is a highly nontrivial task which is beyond the scope of the present study. In this paper, in order to treat the excitation of a highly charged ion in collisions with a many-electron atom, we shall use a simplified picture of the excitation process which consists of the following main "ingredients." First, the electron of the ion is regarded as the only particle having the dynamical degrees of freedom which are described by the wave equation. Second, the nuclei of the ion and the atom are described as classical particles which move along given (straight-line) trajectories and are just the sources of the external electromagnetic field acting on the electron of the ion. Third, the influence of the electrons of the atom on the excitation process will be estimated within the first order perturbation theory in the interaction between the electron of the ion and the atom. It will be shown that, unless the collision energy reaches relatively high values (which will not be of interest for the present study), the role of the atomic electrons in the excitation of a very tightly bound electron in the ion is just of minor importance and they can simply be neglected. Thus, within the simplified picture the process of the excitation of the electron of the ion is effectively reduced to a three-body problem of the motion of the electron in the electromagnetic fields generated by two pointlike classical particles.

It is convenient to treat the excitation process using a reference frame K in which the nucleus of the ion is at rest. We take the position of the nucleus as the origin and assume that in the frame K the nucleus of the atom moves along a straight-line classical trajectory $\mathbf{R}(t)=\mathbf{b}+\mathbf{v}t$, where $\mathbf{b}=(b_x,b_y,0)$ is the impact parameter, $\mathbf{v}=(0,0,v)$ is the collision velocity, and t is the time.

Disregarding for the moment the electrons of the atom, the Dirac equation for the electron of the ion reads

$$i\frac{\partial \Psi}{\partial t}=[\hat{H}_0+\hat{W}(t)]\Psi, \tag{1}$$

where

$$\hat{H}_0 = c\boldsymbol{\alpha}\cdot\hat{\mathbf{p}} - \frac{Z_p}{r} + \beta c^2 \tag{2}$$

is the electronic Hamiltonian for the undistorted ion. Further,

$$\hat{W}(t) = -\Phi(\mathbf{r},t) + \boldsymbol{\alpha}\cdot\mathbf{A}(\mathbf{r},t) \tag{3}$$

is the interaction between the electron of the ion and the nucleus of the atom, where $\boldsymbol{\Phi}$ and $\mathbf{A}$ are the scalar and vector potentials of the electromagnetic field generated by the atomic nucleus. In the Lorentz family of gauges these potentials are normally taken in the Lienard-Wiechert form (see, e.g., [4,10])

$$\Phi(\mathbf{r},t) = \frac{\gamma Z_t}{s},$$

$$\mathbf{A}(\mathbf{r},t) = \frac{\mathbf{v}}{c}\Phi(\mathbf{r},t). \tag{4}$$

In the above equations $\hat{\mathbf{p}}$ is the electron momentum, $\boldsymbol{\alpha}=(\alpha_x,\alpha_y,\alpha_z)$ and β are the Dirac matrices, Z_p and Z_t are the charges of the nucleus of the ion and the nucleus of the atom, respectively, $\mathbf{r}=(x,y,z)$ are the electron coordinates with respect to the nucleus of the ion, $\mathbf{s}=(s_x,s_y,s_z)=[x-b_x, y-b_y, \gamma(z-vt)]$, and $\gamma=1/\sqrt{1-v^2/c^2}$ is the collisional Lorentz factor.

The prior form of the semiclassical transition amplitude is given by

$$a_{fi}(\mathbf{b}) = -i\int_{-\infty}^{+\infty} dt\langle\Psi^{(-)}(t)|(\hat{H} - i\partial/\partial t)\chi_i(t)\rangle. \tag{5}$$

In Eq. (5) $\Psi^{(-)}(t)$ is the solution of the full Dirac equation (1) and $\chi_i(t)$ is the solution of

$$i\frac{\partial\chi_i}{\partial t} = [\hat{H}_0 + V(t)]\chi_i, \tag{6}$$

where $V(t)$ is a distortion potential. The initial condition reads $\chi_i(t\to-\infty)\to\psi_i\exp(-i\varepsilon_i t)$, where ψ_i is the (undistorted) initial state of the electron of the ion with an energy ε_i.

In what follows it will be more convenient to work with the transition amplitude in the momentum space $S_{fi}(\mathbf{Q})$ which is related to the amplitude (5) by the two-dimensional Fourier transformation

$$S_{fi}(\mathbf{Q}) = \frac{1}{2\pi}\int d^2\mathbf{b}\, a_{fi}(\mathbf{b})\exp(i\mathbf{Q}\cdot\mathbf{b}). \tag{7}$$

In Eq. (7) $\mathbf{Q}$ is the two-dimensional transverse part of the momentum transfer $\mathbf{q}$ to the ion, which is perpendicular to the velocity $\mathbf{v}$, $\mathbf{Q}\cdot\mathbf{v}=0$.

A. First order approximation

The first order transition amplitude is obtained from Eqs. (5)–(7) by replacing the states $\chi_i(t)$ and $\Psi^{(-)}(t)$ by the undistorted initial, ψ_i, and final, ψ_f, states of the electron in the ion as follows:

$$\chi_i(t) = \psi_i(\mathbf{r})\exp(-i\varepsilon_i t),$$

$$\Psi^{(-)}(t) = \psi_f(\mathbf{r})\exp(-i\varepsilon_f t), \tag{8}$$

where ε_f is the energy of the electron in the final state of the ion.

Using Eqs. (3), (4), (7), and (8), the first order amplitude is obtained to be

$$S_{fi}^{(1)}(\mathbf{Q}) = \frac{2iZ_t}{v}\frac{1}{q'^2}\left(\langle\psi_f|\exp(i\mathbf{q}\cdot\mathbf{r})|\psi_i\rangle - \frac{v}{c}\langle\psi_f|\exp(i\mathbf{q}\cdot\mathbf{r})\alpha_z|\psi_i\rangle\right), \tag{9}$$

where the momentum $\mathbf{q}$, which is transferred to the electron of the ion in the collision, is given by

$$\mathbf{q} = (q_x,q_y,q_z) = (\mathbf{Q};q_z),$$

$$q_z = \frac{\varepsilon_f - \varepsilon_i}{v}, \tag{10}$$

and

$$\mathbf{q}' = (q_x,q_y,q_z/\gamma) = (\mathbf{Q};q_z/\gamma). \tag{11}$$

Expression (9) presents the first order amplitude in its most frequently used form (see, e.g., [3,4,6,8,9]). Note that the first and second parts of Eq. (9) arise due to the contributions of the coupling of the electron's charge and current densities to the scalar and vector potentials (4), respectively.

For the goals of the present paper it is useful to cast the first order amplitude into a different form. This can be most conveniently done by using the charge conservation condition for the transition density and the current of the electron of the ion. This condition, expressed as the continuity equation in the momentum space (see, e.g., [7], p. 219), reads

$$\frac{\varepsilon_i - \varepsilon_f}{c}\langle\psi_f|\exp(i\mathbf{q}\cdot\mathbf{r})|\psi_i\rangle + \langle\psi_f|\exp(i\mathbf{q}\cdot\mathbf{r})\mathbf{q}\cdot\boldsymbol{\alpha}|\psi_i\rangle = 0. \tag{12}$$

Using Eq. (12) one can replace the first term in parentheses in Eq. (9) and obtain

$$S_{fi}^{(1)}(\mathbf{Q}) = \frac{2iZ_t c}{v^2}\frac{1}{q'^2}\frac{1}{q_z}\left(\langle\psi_f|\exp(i\mathbf{q}\cdot\mathbf{r})(q_x\alpha_x + q_y\alpha_y)|\psi_i\rangle + \frac{1}{\gamma^2}\langle\psi_f|\exp(i\mathbf{q}\cdot\mathbf{r})q_z\alpha_z|\psi_i\rangle\right). \tag{13}$$

Note that the change in the form of the first order transition amplitude [compare Eq. (13) with Eq. (9)] corresponds to the following gauge transformation of the potentials of the electromagnetic field of the nucleus of the atom:

$$\Phi(\mathbf{r},t) \to \Phi'(\mathbf{r},t) = \Phi(\mathbf{r},t) - \frac{1}{c}\frac{\partial f}{\partial t},$$

$$\mathbf{A}(\mathbf{r},t) \to \mathbf{A}'(\mathbf{r},t) = \mathbf{A}(\mathbf{r},t) + \boldsymbol{\nabla} f, \tag{14}$$

where $\Phi(\mathbf{r},t)$ and $\mathbf{A}(\mathbf{r},t)$ are given by Eqs. (4) and the gauge function f is chosen according to

$$f = -\frac{c}{v} Z_t \ln(vs + vs_z). \tag{15}$$

The transformation (14) and (15) leads to the gauge in which the scalar potential of the atomic nucleus is zero and the electromagnetic field generated by the nucleus of the atom is described solely by the vector potential

$$\Phi'(\mathbf{r},t) = 0,$$

$$\mathbf{A}'(\mathbf{r},t) = -\frac{cZ_t}{vs}\left(\frac{s_x}{s+s_z}; \frac{s_x}{s+s_z}; \frac{1}{\gamma}\right). \tag{16}$$

The continuity equation (12) holds provided ψ_i and ψ_f are exact eigenstates of the Hamiltonian $\hat{H}_0$. Therefore, if exact Coulomb-Dirac wave functions are employed to describe the initial and final undistorted states of the electron in the ion, the first order transition amplitude is gauge independent and both expressions (9) and (13) for the amplitude are fully equivalent.

1. Effect of the atomic electrons

In general, there are two points which may invalidate the application of the simple first order three-body model described in the previous section. The first one is the presence of the electrons of the atom. The second point is that in collisions with atoms having relatively large atomic numbers the first order approaches may fail because of the strong interaction between the electron of the ion and the nucleus of the atom. Both points limit the range of the applicability of the simple three-body perturbation theory and demand the development of more sophisticated approaches. We postpone the discussion of the second point to the next subsections and here briefly consider the effects of the atomic electrons.

In ion-atom collisions the motion of the electron of the ion can also be affected by its interaction with atomic electrons. According to theories, in which the interaction between the ion and the atom is treated within the first order approximation, the influence of the atomic electrons on the electron transitions in the ion is twofold (see, e.g., [11,12]). On one hand, when in the ion-atom collisions the electrons of the atom remain in the same initial (ground) state, their presence leads to a partial screening of the field of the atomic nucleus. This effect of the atomic electrons is called screening and it reduces the excitation cross sections compared to results of a theoretical analysis which does not take these electrons into account. On the other hand, because of the collision the electrons of the atom can also make transitions. These transitions lead to the additional contribution to the cross sections for the excitation of the electron of the ion. Such an effect is called "antiscreening."

In collisions between very heavy hydrogenlike ions and not too heavy many-electron atoms the influence of the atomic electrons on the excitation process is not very important unless the collision energy reaches sufficiently high values. Indeed, in collisions at $\gamma \sim 1$ the excitation of the electron, which is very tightly bound in a heavy ion, occurs mainly at so small impact parameters where the atomic electrons are not able to effectively screen the field of the atomic nucleus (see for illustration, Fig. 1). Concerning the contribution to the excitation of the electron of the ion from the antiscreening effect, one should note that this process, viewed as a function of the collision energy, has a threshold (see, e.g., [11,12]). Below the threshold, the process has a vanishingly small probability. But even above the threshold, the contribution of the antiscreening to the cross section for the excitation of the electron of a highly charged ion is roughly proportional to Z_t, whereas the contribution to the cross section given by the interaction with the nucleus of the atom is proportional to Z_t^2. Therefore, in the case of collisions with many-electron atoms, where $Z_t \gg 1$, the contribution of the antiscreening effect to the excitation of a tightly bound electron always remains of minor importance.

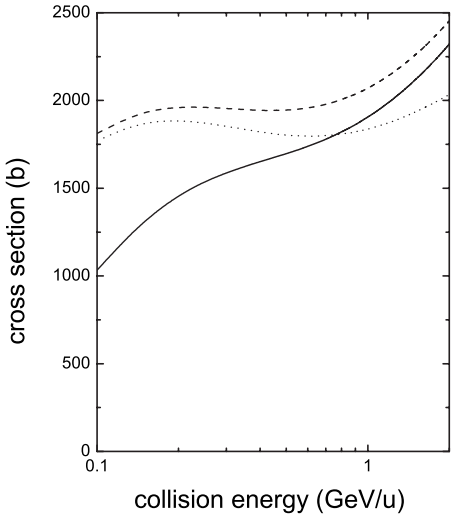

FIG. 1. Cross section for the total excitation into the $2p_{3/2}$ states of Bi^{82+} $(1s_{1/2})$ in collisions with krypton $(Z_t=36)$ given as a function of the collision energy. Dashed and dotted curves display results of the first order calculations without and with taking into account the screening effect of the atomic electrons, respectively. For more information, results of the calculation with the eikonal amplitude (28) are also shown (solid curve).

B. Eikonal approximations

Below we concentrate our attention on collisions at relatively low energies where the influence of the atomic electrons on the excitation of the ion is weak and can be ignored. At such energies, however, the interaction between the electron and the nucleus of the atom may be strong enough to expect noticeable deviations from predictions of the first order calculation.

1. Symmetric eikonal approximation

In an attempt to obtain a better description of the interaction between the electron of the ion and the nucleus of the atom we now approximate the initial and final states in Eq. (5) by χ_i and χ_f, respectively, where

$$\chi_i(t) = \psi_i(\mathbf{r})(vs + \mathbf{v}\cdot\mathbf{s})^{-i\eta_t} \exp(-i\varepsilon_i t),$$

$$\chi_f(t) = \psi_f(\mathbf{r})(vs - \mathbf{v}\cdot\mathbf{s})^{i\eta_t}\exp(-i\varepsilon_f t), \tag{17}$$

with $\eta_t = Z_t/v$. The (prior form of the) semiclassical transition amplitude is now given by

$$a_{fi}^{eik}(\mathbf{b}) = -i\int_{-\infty}^{+\infty} dt\langle\chi_f^{\dagger}(t)|\hat{W}_d(t)\chi_i(t)\rangle. \tag{18}$$

Using the explicit form of the Hamiltonian $\hat{H}$ one can show that the action of the distortion interaction $\hat{W}_d(t) = \hat{H} - i\frac{\partial}{\partial t}$ on the initial state is defined according to

$$\hat{W}_d\chi_i = -\frac{cZ_t}{v}(vs + \mathbf{v}\cdot\mathbf{s})^{-i\nu_t}\left(\frac{s_x\alpha_x + s_y\alpha_y}{s + s_z} + \frac{\alpha_z}{\gamma}\right) \times\psi_i\exp(-i\varepsilon_i t). \tag{19}$$

Taking the above expression into account, the transition amplitude in the impact parameter space (19) reads

$$a_{fi}^{eik}(\mathbf{b}) = i\frac{Z_t c}{v}\int_{-\infty}^{+\infty} dt\exp[i(\varepsilon_f - \varepsilon_i)t]\int d^3\mathbf{r}(vs_{\perp})^{-2i\nu_t}\psi_f^{\dagger}(\mathbf{r}) \times\left(\frac{s_x\alpha_x + s_y\alpha_y}{s + s_z} + \frac{\alpha_z}{\gamma}\right)\psi_i(\mathbf{r}), \tag{20}$$

where $s_{\perp} = \sqrt{s_x^2 + s_y^2}$. The corresponding transition amplitude written in the momentum space is then given by

$$S_{fi}^{eik}(\mathbf{Q}) = \frac{iZ_t c}{2\pi v^2\gamma}\left(\int d^3\mathbf{s}(vs_{\perp})^{-2i\nu_t}\frac{\exp(-i\mathbf{q}'\cdot\mathbf{s})}{s}\frac{s_x}{s + s_z}\langle\psi_f|\exp(i\mathbf{q}\cdot\mathbf{r})\alpha_x|\psi_i\rangle + \int d^3\mathbf{s}(vs_{\perp})^{-2i\nu_t}\frac{\exp(-i\mathbf{q}'\cdot\mathbf{s})}{s}\frac{s_y}{s + s_z}\langle\psi_f|\exp(i\mathbf{q}\cdot\mathbf{r})\alpha_y|\psi_i\rangle + \int d^3\mathbf{s}(vs_{\perp})^{-2i\nu_t}\frac{\exp(-i\mathbf{q}'\cdot\mathbf{s})}{s}\frac{1}{\gamma}\langle\psi_f|\exp(i\mathbf{q}\cdot\mathbf{r})\alpha_z|\psi_i\rangle\right). \tag{21}$$

Performing in Eq. (21) the integration over the vector $\mathbf{s}$ we obtain the following result for the transition amplitude:

$$S_{fi}^{eik}(\mathbf{Q}) = \frac{2iZ_t c}{v^2}\frac{1}{q'^2 q_z}\left(\frac{q'}{2}\right)^{2i\nu_t}\Gamma^2(1 - i\nu_t) \times\left((1 - i\nu_t)\,{}_2F_1(1 - i\nu_t, i\nu_t; 2; Q^2/q'^2)\langle\psi_f|\exp(i\mathbf{q}\cdot\mathbf{r}) \times(q_x\alpha_x + q_y\alpha_y)|\psi_i\rangle + {}_2F_1(1 - i\nu_t, i\nu_t; 1; Q^2/q'^2) \times\frac{1}{\gamma^2}\langle\psi_f|\exp(i\mathbf{q}\cdot\mathbf{r})q_z\alpha_z|\psi_i\rangle\right), \tag{22}$$

where $\Gamma(z_1)$ and ${}_2F_1(a,b;c;z_2)$ are the Gamma function and hypergeometric function, respectively (see, e.g., [13]).

2. Correspondence between the symmetric eikonal and first order approximations

Taking into account that $\lim_{\nu_t\to 0}\Gamma(1 - i\nu_t) = 1$ and $\lim_{\nu_t\to 0}\,{}_2F_1(1 - i\nu_t, i\nu_t; m; z) = 1$ (see [13]) we find that in the limit $\nu_t \to 0$ ($\nu_t \ll 1$) the eikonal amplitude (22) reduces to the first order amplitude (13). If, in addition, the initial and final states of the electron of the ion are described by the Coulomb-Dirac states, the amplitudes (9) and (13) are fully equivalent and, thus, the eikonal amplitude (22) in the limit $\nu_t \ll 1$ reduces also to the "standard" first order amplitude (9).

The fact that in the limit $\nu_t \to 0$ the eikonal amplitude goes over directly to the first order amplitude in the form (13) [and not to Eq. (9)] is not surprising. Such a behavior of the eikonal amplitude can be understood by remarking that the introduction of the eikonal distortion factor into the initial electron state is similar to performing the gauge transformation (14) and (15).

3. Symmetric eikonal approximation and spin-flip transitions

As we have seen, in the limit $\nu_t \to 0$ the symmetric eikonal result for the excitation amplitude does go over into the first order one. However, when the parameter ν_t increases the amplitude (22) yields reasonable results only for transitions not involving electron spin flip while its results for spin-flip transitions start to deviate too strongly from the first order ones rapidly reaching spuriously large values (see for illustration, Fig. 2).

It is not difficult to trace the formal root of this problem. The magnetic component of the electromagnetic field created by the nucleus of the atom in the rest frame of the ion has nonzero components only in the plane perpendicular to the velocity $\mathbf{v}$. However, according to the relativistic first order approximation (13) proper results for the spin-flip transitions are obtained due to the delicate inter-relation (near cancellation) between the transition matrix elements involving, in general, all the components of the electron transition current. In the symmetric eikonal amplitude (22) the transverse (x,y) and the longitudinal (z) components of the electron transition current are modified by the distortion factors. These factors coincide only at $\nu_t \ll 1$ and become rather different when ν_t increases. The latter point leads to the violation of the delicate near cancellation mentioned above and results in strongly overestimated values of the cross sections for spin-flip transitions [14].

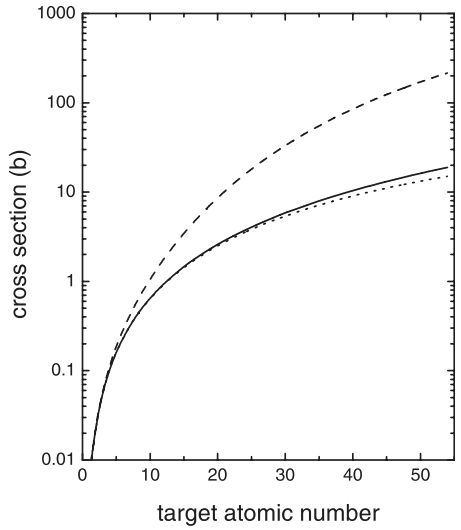

FIG. 2. Cross section for the excitation of 200 MeV/u U^{91+} $(1s_{1/2}(+1/2))$ into the $2s_{1/2}(-1/2)$ state given as a function of the atomic number of the target. Solid curve: results of the first order calculation. Dashed curve: results of calculations with the amplitude (22). Dotted curve: results of calculations with the amplitude (28).

One should also note that the symmetric eikonal approximation is well known to yield very unsatisfactory results for the electron capture occurring in relativistic collisions (see for discussions, e.g., [3–5]). One has to emphasize, however, the important difference between the reasons of the failures of the symmetric eikonal model in the cases of capture and excitation. Namely, since the exact solution of the three-body problem (an electron moving in the fields of two colliding nuclei) is not available, in the case of capture the initial and final undistorted states of the electron in the symmetric eikonal approximation are described by wave functions belonging to the different Hamiltonians. As a result, the difficulties with the application of the symmetric eikonal approximation in the case of electron capture are also closely related to the general problem of gauge dependence [15]. In contrast, in the case of excitation the initial and final undistorted states of the electron belong to the same Hamiltonian and by using the exact Coulomb-Dirac states the gauge dependence of the first-order excitation cross section can be avoided. Therefore, in the case of excitation the problem with the symmetric eikonal approximation is much less severe than in the case of capture.

The symmetric eikonal approximation has been a very useful tool in the applications to nonrelativistic ion-atom collisions [16]. Moreover, the version of the symmetric eikonal model based on the nonrelativistic description of the electron turned out to be quite successful in the description of collisions between relativistically moving highly charged ions and very light targets [17,18]. The general and very valuable advantage of the eikonal-like approaches is that, on one hand, they enable one in many cases to reach a much better description of the collision process compared to the first Born approximation and, on the other hand, are almost as simple and not time consuming in applications as the latter. Therefore, keeping this in mind and taking into account that the problem with the symmetric eikonal approximation in the case of the excitation does not seem to be severe, it is worth trying just to "fix" the amplitude (22) without resorting to more sophisticated (and more complicated) approaches.

It is natural to set the following conditions for the corrected amplitude. (i) This amplitude should be free of the above discussed problem with the description of transitions involving electron spin flip. (ii) In the case of weak perturbations $(\nu_t \ll 1)$ this amplitude should go over into the first order one given by Eq. (13). (iii) At larger perturbations for transitions not involving electron spin flip [such as, e.g., $1s_{1/2}(1/2) \to 2s_{1/2}(1/2)$] the corrected amplitude should yield results close to those obtained with the amplitude (22).

As was already mentioned, there exists the symmetric eikonal model for collisions at relativistic impact energies employing the Schrödinger-Pauli equation to treat the electron motion. In this model, which is briefly described in the next section, the problem with spin-flip transitions does not arise at all. Therefore, it seems to be reasonable to set one more condition that (iv) both the corrected eikonal amplitude obtained with the Dirac equation and the eikonal amplitude based on the Schrödinger-Pauli equation should yield close results for the excitation of not very heavy ions where the motion of the electron in the initial and final undistorted states of the ion is only weakly affected by the relativistic effects.

4. Symmetric eikonal approximation for nonrelativistic electron description

In this subsection we very briefly consider the symmetric eikonal model for the nonrelativistic electron [19,20]. In this model the potentials Φ and $\mathbf{A}$ are taken in the fully relativistic form but the motion of the electron is treated nonrelativistically by using the Schrödinger-Pauli equation. In the case of the electron, which moves in the field of the ionic nucleus and is also subjected to the field of a relativistically moving atomic nucleus, this equation reads

$$i\frac{\partial \Psi}{\partial t} = [\hat{H}_0 + \hat{W}(t)]\Psi, \tag{23}$$

where

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{Z_p}{r} \tag{24}$$

is the nonrelativistic electronic Hamiltonian for the undistorted ion. The interaction between the electron of the ion and the nucleus of the atom is now given by

$$\hat{W}(t) = -\Phi(\mathbf{r},t) + \frac{1}{2c}[\mathbf{A}(\mathbf{r},t)\cdot\hat{\mathbf{p}} + \hat{\mathbf{p}}\cdot\mathbf{A}(\mathbf{r},t)] + \frac{\mathbf{A}^2(\mathbf{r},t)}{2c^2} + \frac{1}{2c}\boldsymbol{\sigma}\cdot\mathbf{H}(\mathbf{r},t), \tag{25}$$

where $\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ are the Pauli matrices, Φ and $\mathbf{A}$ are the scalar and vector potentials defined by Eq. (4), and $\mathbf{H}=\boldsymbol{\nabla}\times\mathbf{A}$ is the magnetic part of the electromagnetic field generated by the atomic nucleus in the rest frame of the ion. For

definiteness we shall assume that initially the electron spin is directed along the collision velocity $\mathbf{v}$.

At this place a brief remark concerning the term $\sim \mathbf{A}^2/2c^2$ of the Schrödinger-Pauli equation may be appropriate. In the consideration given in a well known paper [20] this term was found to dominate in the transition amplitude at asymptotically high impact energies and to result in a wrong asymptotic behavior of the cross sections. In order to overcome this problem it was proposed in [20] to add into the Schrödinger-Pauli equation a term proportional to $-\Phi^2/2c^2$. However, it can be shown (see [21]) that the canonic form of the Schrödinger-Pauli equation [Eqs. (23)–(25)] is quite capable of yielding a proper description for a nonrelativistic electron in the field generated by a relativistically moving charge and must not be modified. It can be also shown (see [21]) that the problem with an unphysical contribution from the term $\sim \mathbf{A}^2$ obtained in the treatment of [20] is caused by the fact that the interaction (25) (adopted in [20] as the starting expression for the *first* order perturbation—see formula (3.1) of [20]) as well as the interaction modified by adding the term $\sim -\Phi^2/2c^2$ [see formula (3.2) of [20]], after being "sandwiched" in the transition amplitude between the states of the Hamiltonian $\hat{H}_0$, becomes not compatible with the continuity equation for the electron transition charge and current densities and thus violates the conservation of the electric charge. In the present paper we shall not consider this point further and for its very detailed discussion refer to [21]. Here we just mention that, as is known [22], in the symmetric eikonal approximation the problem with the contribution from the term $\sim \mathbf{A}^2$ does not arise.

In the symmetric eikonal approximation the amplitude for transitions without spin flip reads [22]

$$S_{fi}^{no\text{-}flip}(\mathbf{Q}) = \frac{2iZ_t c}{v^2 q_z}\frac{1}{q'^2}\left(\frac{q'}{2}\right)^{2i\nu_t}\Bigg((1-i\nu_t)\Gamma^2(1-i\nu_t)\,{}_2F_1(1-i\nu_t, i\nu_t; 2; Q^2/q'^2)\langle\varphi_f|\exp(i\mathbf{q}\cdot\mathbf{r})(q_x\hat{p}_x + q_y\hat{p})|\varphi_i\rangle$$
$$+\Gamma^2(1-i\nu_t)\,{}_2F_1(1-i\nu_t, i\nu_t; 1; Q^2/q'^2)\frac{1}{\gamma^2}\langle\varphi_f|\exp(i\mathbf{q}\cdot\mathbf{r})q_z\hat{p}_z|\varphi_i\rangle$$
$$+\Gamma^2(1-i\nu_t)\,{}_2F_1(1-i\nu_t, i\nu_t; 1; Q^2/q'^2)\frac{q'^2}{2}\langle\varphi_f|\exp(i\mathbf{q}\cdot\mathbf{r})|\varphi_i\rangle$$
$$+\Gamma(1-2i\nu_t)\,{}_2F_1(0.5-i\nu_t, i\nu_t; 1; Q^2/q'^2)\frac{\pi\nu_t q' q_z}{2\gamma}\langle\varphi_f|\exp(i\mathbf{q}\cdot\mathbf{r})|\varphi_i\rangle\Bigg), \tag{26}$$

where φ_i and φ_f are the initial and final eigenstates of the Schrödinger Hamiltonian (24) [23] and q_z is given by Eq. (10), where the relativistic energies ε_i and ε_f have to be replaced by the corresponding nonrelativistic values. Further, one can show that the amplitude for electron spin-flip transitions in this model is given by

$$S_{fi}^{flip}(\mathbf{Q}) = -\frac{iZ_t}{c^2}\frac{q_x + iq_y}{q'^2}\left(\frac{q'}{2}\right)^{2i\nu_t}(1-i\nu_t)\Gamma^2(1-i\nu_t)$$
$$\times\,{}_2F_1(1-i\nu_t, i\nu_t; 2; Q^2/q'^2)\langle\varphi_f|\exp(i\mathbf{q}\cdot\mathbf{r})|\varphi_i\rangle. \tag{27}$$

By setting $\nu_t = 0$ in Eq. (27) we recover the corresponding first order amplitude for the spin-flip transitions obtained by using the Schrödinger-Pauli equation. It is obvious from the very structure of the amplitude (27) that there is no problem with the description of spin-flip transitions also at finite values of ν_t. As calculations show, in the limit $\nu_t \ll 1$ the cross sections for spin-flip transitions obtained with the amplitude (27) practically coincide with those given by the corresponding first order approximation. At larger ν_t the eikonal model predicts that the spin-flip cross sections increase slower with the increase in ν_t compared to the results of the first order calculation [for illustration, see Fig. 3(a)].

The above discussed symmetric eikonal model is based on the nonrelativistic electron description and, therefore, can be sufficiently accurate only when applied to ions with not too high values of Z_i ($Z_i \lesssim 30-40$). Besides, being an eikonal-type model, it is expected in general to yield good results only provided $\nu_t \lesssim 1$, i.e., at not too low impact energies where $v \gtrsim Z_t$. On the other hand, the model does not have limitations from the side of high impact energies (see [19,20]): it can formally be applied even at $\gamma \to \infty$ [24]. Thus, the range of the validity of the symmetric eikonal model with the nonrelativistic electron description to treat the excitation by collisions with pointlike charges Z_t is restricted to $Z_t \lesssim v < c$ and $Z_i \lesssim 30-40$.

5. "Modified" eikonal amplitude

The electromagnetic force, exerted by the nucleus of the moving atom on the electron of the ion, acts both in the plane perpendicular to the collision velocity (the transverse direction) and parallel (or antiparallel) to this velocity (the longitudinal direction). However, as is well known, in fast collisions the most important part of this force is normally the transverse force. In particular, it is the transverse part of the electric field of the atomic nucleus whose action on the electron of the ion in collisions with sufficiently small impact

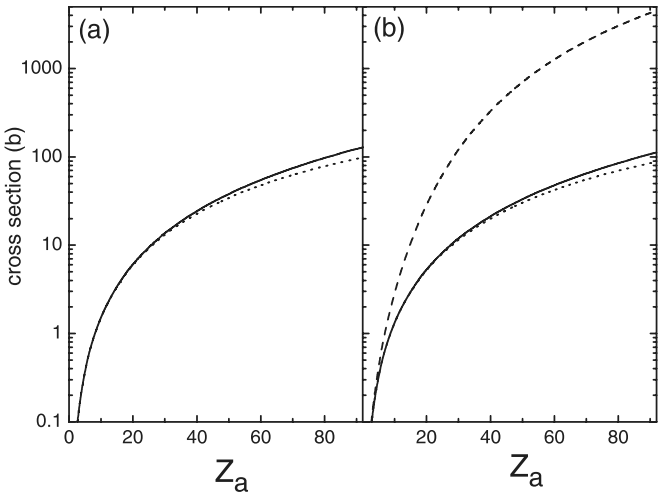

FIG. 3. Cross section for the excitation of 200 MeV/u $Zr^{39+}(1s_{1/2}(1/2))$ into the $2s_{1/2}(-1/2)$ state in collisions with a pointlike charge Z_a obtained by using the Schrödinger-Pauli equation (a) and the Dirac equation (b). (a) Dotted curve: results of calculations with the amplitude (27). Solid curve: results of the first order calculation [the calculation with Eq. (27) where in the eikonal distortion factor ν_t is set to zero]. (b) Solid curve: results of the first order calculation with the amplitude (13). Dashed and dotted curves: results of the calculations with the amplitudes (22) and (28), respectively.

parameters may become effectively too strong invalidating the application of the first Born approximation. Therefore, it is mostly the "transverse" part of the interaction between the electron and the atomic nucleus which may need a treatment beyond the framework of the first order approximation.

In this respect it is worth noting that the only (but important) difference between the symmetric eikonal amplitudes (20) and (21) and their first order counterpart is the presence of the factor $(vs_\perp)^{-2i\nu_t}$ in Eqs. (20) and (21). This factor depends only on the transverse component of the vector $\mathbf{s}$ and using the Fourier transformation it can be shown to result in the two-dimensional virtual momentum transfer which is perpendicular to the collision velocity and describes the additional (with respect to the first order consideration) exchange of virtual photons between the particles on the intermediate stage of the collision process. Because of its manifestly transverse character the factor $(vs_\perp)^{-2i\nu_t}$ *per se* neither carries any relativity effects nor attempts to improve the description of the interactions in the transverse and longitudinal directions in a harmonious manner.

According to the Schrödinger-Pauli equation electron transitions with and without spin flip can always be separated and the spin may be affected by the magnetic field only. In the relativistic description the situation is quite different. In particular, the electron spin couples both to the magnetic and electric parts of the electromagnetic field generated in the collision. In contrast to the magnetic field, the electric field has nonzero components not only in the plane perpendicular to the collision velocity but also parallel to it.

The subtleties inherent to the relativistic electron description put in general much more demand to the quality of collision models, especially those which go beyond the first order approximation. Compared to the first order approach the symmetric eikonal model attempts to improve the treatment of the interaction between the electron and the field of the atomic nucleus focusing on the transverse direction without taking much care about the longitudinal one. This partially violates that subtle harmony in the description of the interaction of the relativistic electron with the transverse and longitudinal components of the electric field which is present in the first order approximation. It seems plausible to assume that the problem with spin-flip transitions which the symmetric eikonal model faces being applied to the Dirac electron is directly related to this and such an assumption is indeed supported by the fact that the problem actually disappears in collisions at sufficiently high γ in which the longitudinal component of the electric field generated by the moving atomic nucleus becomes very small.

The observation made in Sec. II B 3 about the formal root of the problem with treating spin-flip transitions by using the amplitude (22) suggests that one can try to improve the amplitude (22) by simply "correcting" the eikonal distortion factors coupled to the x, y, and z components of the electron transition current in such a way that all of them become equal. Taking into account what has been said in the above paragraphs of this section one may try to improve the description of the collision by altering in the amplitude (22) the eikonal distortion factor coupled to the z component of the electron transition current so that this distortion factor becomes equal to those for x and y components [25]. Note also that such a procedure minimizes possible changes in the eikonal distortion factors in the amplitude (22).

With this change we get the following amplitude:

$$S_{fi}^{m}(\mathbf{Q}) = \frac{2iZ_t c}{v^2}\frac{1}{q'^2 q_z}\left(\frac{q'}{2}\right)^{2i\nu_t} \times \Gamma^2(1-i\nu_t)(1-i\nu_t)_2F_1(1-i\nu_t, i\nu_t; 2; Q^2/q'^2) \times \left(\langle\psi_f|\exp(i\mathbf{q}\cdot\mathbf{r})(q_x\alpha_x + q_y\alpha_y)|\psi_i\rangle + \frac{1}{\gamma^2}\langle\psi_f|\exp(i\mathbf{q}\cdot\mathbf{r})q_z\alpha_z|\psi_i\rangle\right). \quad (28)$$

Enforcing the distortion factors to be equal, of course, does not mean that unphysical equivalence between the transverse (x,y) and the longitudinal (z) directions has been tacitly imposed. Indeed, the components of the electron transition current do not enter the amplitude (28) on an equal footing and the asymmetry between these directions is explicitly embodied in Eq. (28) where the z component of the current is multiplied by a factor $1/\gamma^2$ that distinguishes the z direction and reflects the relativistic flattening of the field generated by a fast moving charge.

We have compared results for the excitation of intermediately heavy ions ($Z_i \sim 30-40$) obtained by using the amplitude (28) with results given by the application of the eikonal amplitudes (26) and (27). In all cases tested the amplitude (28) yielded cross section values which were close to results obtained with the amplitudes (26) and (27), including the case of spin-flip transitions (see for illustration, Fig. 3).

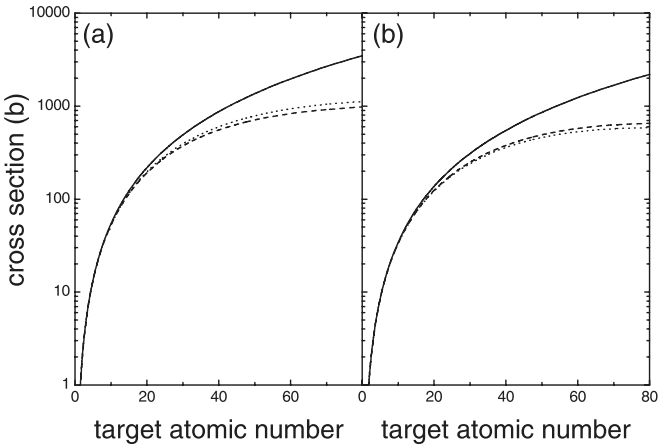

FIG. 4. Cross section for the excitation of 150 MeV/u $U^{92+}(1s_{1/2}(1/2))$ into the $2s_{1/2}(1/2)$ state (a) and into the $2p_{3/2}(3/2)$ state (b) given as a function of the atomic number of the target. Solid curves: results of the calculations with the amplitude (13). Dotted and dashed curves: results of calculations with the amplitudes (28) and (22), respectively.

Concerning the application of the corrected eikonal amplitude to the treatment of the excitation of heavy ions, in which the motion of the electron has to be described by the Dirac equation and where the comparison with the eikonal amplitudes (26) and (27) is no longer relevant, one should note the following. First, as is obvious from the very structure of the amplitude (28), in the limit $\nu_t \to 0$ ($\nu_t \ll 1$) this amplitude reduces to the relativistic first order amplitude (13). Second, at larger ν_t, for which the difference between the amplitudes (28) and (13) begins to become noticeable, the calculations show that the amplitude (28) yields cross sections which increase slower with the increase in the strength of the perturbation compared to the results obtained in the first order approximation. Such a relation between the first order and eikonal results is pretty much in accord with the experience accumulated in the field of energetic ion-atom collisions which tells us that the first order calculations tend to overestimate excitation and ionization or loss cross sections when the perturbation increases.

Further, there is no problem with the application of the amplitude (28) for the description of transitions which involve electron spin flip. For such transitions, in sharp contrast to calculations with the amplitude (22), the amplitude (28) yields cross sections whose values always remain below those obtained from the first order calculations (see for illustration, Figs. 2 and 3). In particular, the relative difference between the relativistic first order and corrected eikonal results for spin-flip transitions is very similar to that between the spin flip cross sections calculated with the amplitude (27) and its first order counterpart (compare, for instance, results in Figs. 2 and 3).

Note also that our test calculations have shown that the amplitudes (22) and (28) give close cross section values for transitions in heavy ions which do not involve electron spin flip (see for illustration, Fig. 4). Besides, at sufficiently high values of γ, both the amplitudes (22) and (28) yield practically identical results for all transitions. The latter is, of course, not surprising since at very high impact energies, because of the presence of the factor $1/\gamma^2$ coupled to the z component of the electron transition current, the difference between Eqs. (22) and (28) simply vanishes.

Thus, summarizing the above discussion one can conclude that the amplitude (28) satisfies all the conditions formulated in Sec. II B 3. Therefore, there are the very substantial grounds to expect the amplitude to be a good approximation for calculating the excitation of heavy ions by relativistic collisions with point like charges Z_t when the effective perturbation strength is not too strong, $\nu_t = Z_t/v \lesssim 1$.

III. RESULTS AND DISCUSSION

Experimental data for the excitation of relativistic heavy hydrogenlike ions were reported in [8,9] for collisions of 82 and 119 MeV/u $Bi^{82+}(1s)$ with solid state targets of carbon, aluminum, and nickel. As was mentioned in [9], the accuracy of the experimental data for the 82 MeV/u projectiles was substantially affected by the electron capture process which, because of the very high projectile charge, is still strong at this impact energy. Therefore, in what follows we restrict a comparison of our theoretical results only to the excitation of 119 MeV/u $Bi^{82+}(1s)$.

At this energy the screening effect of the atomic electrons is quite weak. The effective energy threshold for the antiscreening in collisions with $Bi^{82+}(1s)$ is about 140 MeV/u. Therefore, the antiscreening effect is very weak as well and the influence of the atomic electrons on the excitation process can be safely neglected.

In Fig. 5 we show results for the excitation of 119 MeV/u $Bi^{82+}(1s)$ given as a function of the atomic number of the target. Since at this impact energy the influence of the atomic electrons on the excitation process is weak, theoretical results for the cross sections displayed in the figure were obtained by treating the process as a three-body problem which involves the electron of the ion and the nuclei of the ion and atom.

Figure 5 contains two sections. In section (a) dashes and dotted curves show results obtained with the first order amplitude (13) for the excitation of the ion into the states with $n=2, j=1/2$ and $n=2, j=3/2$, respectively, where n is the principal quantum number and j is the total angular momentum of the electron. Dashed and dotted curves in section (b) display results for the same transitions but are calculated with the amplitude (28). In both sections solid curves show the total cross section for the transitions to all the states with $n=2$ obtained with the corresponding amplitudes. Both sections in Fig. 5 also contain the (same set of) experimental data from [8,9].

It is seen in the figure that both the first order and eikonal transition amplitudes yield very close results for the excitation cross sections in collisions with very light atoms ($Z_t \lesssim 10$) where the interaction of the electron with the nucleus of the atom is weak. In collisions with atoms having larger atomic numbers the difference between the predictions of the first order and eikonal approaches starts to appear. When the atomic number of the target increases further, this difference

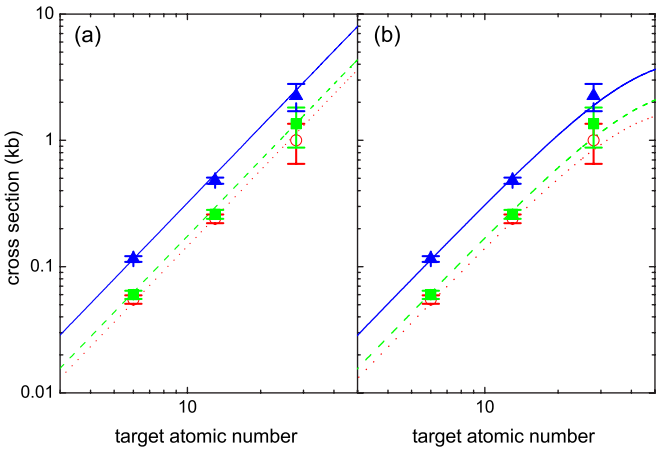

FIG. 5. (Color online) Cross sections for the excitation into states with $n=2, j=1/2$, with $n=2, j=3/2$ and for the total excitation into $n=2$ states of 119 MeV/u $Bi^{82+}(1s_{1/2})$ in collisions with atomic targets whose atomic numbers run between 1 and 54. (a) Results of the first order calculation. Dashed curve: $n=2, j=1/2$; dotted curve: $n=2, j=3/2$; and solid curve: $n=2$. (b) Results obtained with the amplitude (28). Dashed curve: $n=2, j=1/2$; dotted curve: $n=2, j=3/2$; and solid curve: $n=2$. Circles, squares, and triangles (with the corresponding error bars) in (a) and (b) display experimental results from [8,9] for the excitation into the states with $n=2$ and $j=1/2$, $n=2$ and $j=3/2$, and $n=2$, respectively, which were measured in collisions with solid state targets of carbon ($Z_a=6$), aluminum ($Z_a=13$), and nickel ($Z_a=28$).

rapidly increases and reaches almost a factor of two at $Z_t \simeq 50$.

Amongst targets, for which experimental data are available, nickel ($Z_t=28$) has the highest atomic number. For the excitation of 119 MeV/u $Bi^{82+}(1s)$ in collisions with this target the eikonal calculation predicts the reduction of the excitation cross section approximately by 30% compared to the results of the first order model. However, the uncertainty in the experimental point is also about 30% and both the eikonal and first order calculations are in good overall agreement with the experiment (for the first order calculation this was already noticed in [8,9]). Thus, the accuracy of the experimental data does not enable one to make a conclusion about which calculation describes better the experiment.

In Fig. 6 we compare results for the ratio $\sigma(n=2, j=3/2)/\sigma(n=2, j=1/2)$ where $\sigma(n=2, j=1/2)$ and $\sigma(n=2, j=3/2)$ are the cross sections for the excitation to the states with $n=2, j=1/2$ and $n=2, j=3/2$, respectively. The figure shows that, for the excitation to different final states, the deviations between the results, obtained with the first order and eikonal transition amplitudes, are accumulating at a different pace. In particular, the deviation from the first order results is somewhat stronger for the excitation into the states with $n=2, j=3/2$. Note also that, in contrast to the case of the absolute cross sections where the available experimental data do not allow us to prefer one of the two calculations, the experimental data for the cross section ratio seem to be more in favor of the results obtained with the amplitude (28).

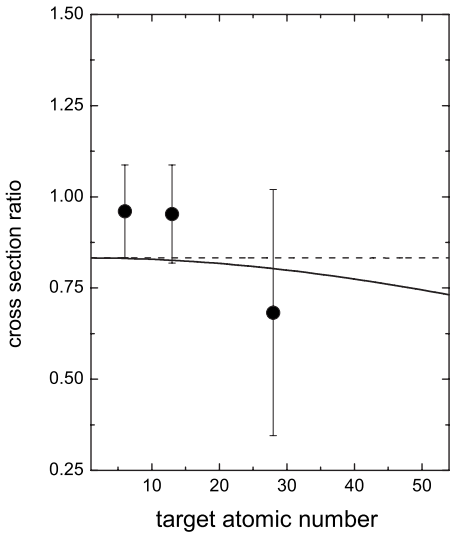

FIG. 6. The ratio $\sigma(n=2, j=3/2)/\sigma(n=2, j=1/2)$ between the cross sections for the excitation of 119 MeV/u $Bi^{82+}(1s_{1/2})$ into the states with $n=2, j=1/2$ and $n=2, j=3/2$. The ratio is given as a function of the atomic number of the target. Dashed line: results of the first order calculation. Solid curve: results obtained with the amplitude (28). Circles with error bars: experimental data from [8,9].

IV. CONCLUSIONS

We have considered the excitation of highly charged hydrogenlike ions in collisions with many-electron atoms. We have discussed two models in which the interaction between the electron of the ion and the atom is treated within first order perturbation theory and also proposed a model which goes beyond the first order approximation.

In the more simple of the first order models the presence of the electrons of the atom is ignored. In the second of these models the screening effect of the atomic electrons is taken into account. In agreement with the general expectations this effect was found to become of importance only when the collision energy (per nucleon) reaches sufficiently large values.

Experimental data on the excitation of very heavy ions are available only for relatively low collision energies. At these energies, which were of main interest for the present study, the role of the atomic electrons is of minor importance and their influence on the excitation process can be neglected. At these energies, however, our calculations suggest that the deviations from predictions of the first order consideration are much more substantial than it was expected in the earlier studies of the excitation process [8,9].

The transition amplitude (28), proposed in the paper for calculating excitation cross sections, has rather a simple form. As a result, calculations performed with this amplitude are computationally almost as straightforward and not time consuming as the first order calculations. The amplitude (28) represents a corrected version of the amplitude (22). The latter, which was derived within the symmetric eikonal approximation, has been shown to yield unphysical results for spin-flip transitions. Having discussed the source of the problem with the amplitude (22), we have made an attempt to

"fix" it and arrived at the corrected amplitude (28) which has minimum changes with respect to the amplitude (22).

(i) For the excitation of not too heavy ions, in which the electron motion in the initial and final undistorted states of the ion is only weakly influenced by the relativistic effects, the amplitude (28) leads to cross sections which are in reasonable agreement with results of the symmetric eikonal model based on the nonrelativistic electron description. (ii) In the case of weak perturbations $\nu_t \ll 1$ the amplitude (28) goes over into the first order relativistic amplitude (13). (iii) For the excitation of both light and heavy ions the amplitude (28) yields very reasonable results for spin-flip transitions. (iv) Results obtained with the amplitudes (28) and (22) for transitions not involving electron spin flip are quite close and (v) at $\gamma \gg 1$ the amplitudes (28) and (22) actually coincide. All these points, despite the amplitude (28) has not been derived in a rigorous way, lend very substantial support to the use of the amplitude (28) in calculations of the excitation of heavy ions in relativistic collisions.

Calculations with the amplitude (28) suggest that the first order approximation may very substantially overestimate the excitation cross sections. These calculations also predict that for the excitation to different states the deviations from the first order results develop at a different pace. In particular, the pace is different for the states with $n=2, j=1/2$ and $n=2, j=3/2$.

According to our results, the differences between cross section values calculated with the amplitude (28) and obtained in the first order approximation can be rather substantial at the impact energies studied experimentally. However, neither of the calculated cross sections contradicts to the available experimental data. The reason for this is that the experimental data have been reported only for targets not heavier than nickel where the predicted deviations from the first order results lie below 30% and, thus, do not exceed the experimental error bars. In collisions of relativistic highly charged ions with heavier atoms, such as e.g., xenon, the predicted deviations should be already accessible for an experimental verification. Therefore, experimental data for the excitation of relativistic ions in collisions with heavier targets (or for targets such as nickel but with better accuracy) would be very desirable [26].

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[14] One should add that in collisions at $\gamma \gg 1$ the z component of the electron current, being suppressed by the very small factor $1/\gamma^2$, actually does not contribute to transitions including also those accompanied by electron spin flip. As a result, at large values of γ the problem with the symmetric eikonal amplitude (22) disappears. Note, however, that at $\gamma \gg 1$ both the amplitudes (13) and (22) yield practically identical cross sections. Besides, as was already mentioned, in collisions with neutral atoms at such high impact energies the three-body model simply cannot be used. Therefore, in the range of impact energies, where the problem with the amplitude (22) is absent, there is actually no need in this amplitude.
[15] The first Born results for the capture are strongly gauge dependent. In the case of weak perturbations the symmetric eikonal result for the capture reduces to the particular case of the first Born approximation. Because of the gauge dependence results of the latter strongly differ from those yielded by the "standard" Born approximation which was extensively used in calculations.
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[23] The spin degrees of freedom are not included in these states.
[24] The eikonal model has been developed for the excitation of ions by a pointlike charged particle. In collisions of ions with neutral atoms at sufficiently high impact energies the effect of atomic electrons has to be taken into account. In this sense it might seem to be not of much physical significance to speak about the asymptotic behavior of the eikonal model in the limit $\gamma \gg 1$. However, in the case when the excitation of not too heavy ions would be induced by in energetic nuclei the model would remain valid even $\gamma \to \infty$.
[25] Such a change is also suggested by the form of the eikonal

distortion factor in the spin-flip amplitude (27).

[26] In principle, the amplitude (28) can be applied not only to treat excitation but also to evaluate the total cross section for the electron loss from heavy ions. Dr. Ch. Scheidenberger from the GSI (Darmstadt, Germany) has drawn our attention to the fact that there exist experimental data for the electron loss from hydrogenlike and heliumlike ions of uranium in collisions with targets ranging from beryllium till gold at impact energies $\sim 100-200$ MeV/u where the effect of the atomic electrons on the loss process is very weak and the three-body models considered in the present paper can be applied. Our calculations for the total loss cross section have indeed proved that the amplitude (28) has a great advantage over the first order one when the parameter $\nu_t = Z_t/v$ approaches 1. For instance, for the single electron loss from 100 MeV/u $U^{90+}(1s^2)$ in collisions with gold the first Born approximation overestimates the experimental data by an order of magnitude while the eikonal amplitude (28) yields the result which is in agreement with the experiment. The topic of the electron loss will be considered in a forthcoming paper.